Time integration

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1 Equations

1.1 Mass conservation

$$\frac{\partial c_i}{\partial t} = -\vec{\nabla}.\vec{N}_i + R_i \tag{1}$$

with

$$\vec{N}_i = c_i\vec{v} - \sum_j D_{ij}\vec{\nabla}c_j - w_i c_i \vec{\nabla}U \tag{2}$$

1.2 Poisson's equation

$$\vec{\nabla}^2 U + \frac{F}{\epsilon}\sum_i z_i c_i = 0 \tag{3}$$

1.3 Butler-Volmer kinetics

$$v = k_{ox}\exp\left[\frac{\alpha_{ox} nF}{RT}(V-U)\right]c_{red} - k_{red}\exp\left[-\frac{\alpha_{red} nF}{RT}(V-U)\right]c_{ox} \tag{4}$$

2 Time integration

2.1 Two parameter discretization schemes

$$\begin{array}{l} [T]\left(\frac{1+\epsilon}{\Delta t}\left(\left\{x^{t+1}\right\}-\left\{x^{t}\right\}\right)-\frac{\epsilon}{\Delta t_{-1}}\left(\left\{x^{t}\right\}-\left\{x^{t-1}\right\}\right)\right) \\ =\theta\left(([C]+[D]+[M]+[H]+[P])\left\{x^{t+1}\right\}+\{E\}\right) \\ +(1-\theta)\left(([C]+[D]+[M]+[H]+[P])\left\{x^{t}\right\}+\{E\}\right) \end{array} \tag{5}$$

with

- $[T]$ the time matrix
- $[C]$ the convection matrix
- $[D]$ the diffusion matrix
- $[M]$ the migration matrix

- $[H]$ the homogeneous reactions matrix
- $[P]$ the Poisson's equation matrix
- $\{E\}$ the electrode reactions vector
- $\left\{x^{t+1}\right\}$, $\{x^t\}$ and $\left\{x^{t-1}\right\}$ the vector of unknowns at time $t+1$, t and $t-1$

The matrices may depend on the unknowns. The equation holds at the element level as well as the global level.

- $\epsilon = 0,\ \theta = 0:$ explicit
- $\epsilon = 0,\ \theta = 1:$ Euler backwards
- $\epsilon = 0,\ \theta = \frac{1}{2}:$ Crank-Nicolson
- $\epsilon = \frac{1}{2},\ \theta = 1:$ 3 point backwards (this is the one used)

2.2 Newton iterations

Define

$$\begin{array}{rcl} \{\Psi\} & = & \left(\frac{1+\epsilon}{\Delta t}\left[T^{t+1}\right] - \theta\left(\left[C^{t+1}\right] + \left[D^{t+1}\right] + \left[M^{t+1}\right] + \left[H^{t+1}\right] + \left[P^{t+1}\right]\right)\right)\left\{x^{t+1}\right\} - \theta\left\{E^{t+1}\right\} \\ & & -\left(\left(\frac{1+\epsilon}{\Delta t} + \frac{\epsilon}{\Delta t_{-1}}\right)\left[T^t\right] + (1-\theta)\left(\left[C^t\right] + \left[D^t\right] + \left[M^t\right] + \left[H^t\right] + \left[P^t\right]\right)\right)\left\{x^t\right\} - (1-\theta)\left\{E^t\right\} \\ & & +\frac{\epsilon}{\Delta t_{-1}}\left[T^{t-1}\right]\left\{x^{t-1}\right\} \\ & = & \{0\} \end{array} \tag{6}$$

First order Taylor expansion

$$\left\{\Psi^{p+1}\right\} \approx \{\Psi^p\} + \left[\frac{\partial \Psi^p}{\partial X}\right]\{\Delta X^p\} = \{0\} \tag{7}$$

with

$$X = \left\{x^{t+1}\right\}$$

$$\left[\frac{\partial \Psi^p}{\partial X}\right] = \frac{1+\epsilon}{\Delta t}\left([T^p] + \left[\tilde{T}^p\right]\right) - \theta\left([C^p] + \left[\tilde{C}^p\right] + [D^p] + \left[\tilde{D}^p\right] + [M^p] + \left[\tilde{M}^p\right] + [H^p] + \left[\tilde{H}^p\right] + [P^p] + \left[\tilde{P}^p\right] + \left[\tilde{E}^p\right]\right)$$

and

- $\left[\tilde{T}\right]$ the time jacobian
- $\left[\tilde{C}\right]$ the convection jacobian
- $\left[\tilde{D}\right]$ the diffusion jacobian
- $\left[\tilde{M}\right]$ the migration jacobian

- $\left[\tilde{H}\right]$ the homogeneous reactions jacobian
- $\left[\tilde{P}\right]$ the Poisson's equation jacobian
- $\left[\tilde{E}\right]$ the electrode reactions jacobian